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Abstract: Making use of mathematical programming algorithms, a software library (AqLib) has been built for automatically optimising the design and operation of wastewater treatment plants. Currently, AqLib implements seven configurations for nitrogen removal (DN, DN2, RDN, SDN, DRDN, RSDN and DRSDN), five configurations for phosphorous removal (A^2O, Bardenpho, Johannesburg, UCT and MUCT), and the anaerobic digestion process. Moreover, an Internet-based service (AqquaStudy) has been deployed so that AqLib can be remotely accessed from any standard web-browser.

Keywords: Web-based, Wastewater, Mathematical modelling, Optimisation

1. INTRODUCTION

Advances in computer technology have motivated significant changes in the methods that are currently being applied to solve engineering problems in general. Feasibility, robustness and calculation speed are some computing features which have encouraged knowledge being progressively transferred to decision-support software tools. As a result of the explosion of computer technologies, model-based simulation has become an effective tool for decision-makers dealing with complex situations. In this respect, model-based software tools are, more than ever, an essential asset within many water engineering companies in order to support the design and operation of wastewater treatment plants (WWTP). As a result of more stringent regulations for both treated water discharges and sludge disposal, many WWTPs are being retrofitted with modern and complex treatment technologies whose design and operating criteria are not straightforward even for experienced professionals [Larrea et al., 2007]. Likewise, the growing competitiveness in the water industry is pushing companies to refine their current WWTP design and operating manuals with the adoption of new procedures that lead to optimum solutions.

Over the last decades, an intensive research has been focused on the mathematical formulation of all those mechanisms involved in the biological treatment of wastewaters. Nevertheless, owing to the great diversity of model proposals and the inherent complexity of these systems, modellers very soon realised the importance of promoting standardisation so as to establish a common framework around mathematical modelling issues. Thus, the confirmation of the standard IWA ASM models for biological COD and nutrient removal [Henze et al., 2000]) as a valuable tool for predicting the behaviour of activated sludge (AS) systems, have meant a decisive driving force towards the progressive acceptance of model-based techniques within water companies. Later on, drawn by the success of the ASM models, the IWA ADM1 model is published and adopted as standard for dynamic modelling of the anaerobic digestion processes [Batstone et. al., 2002]). Moreover, at present, great efforts are being addressed at providing accurate descriptions for promising technologies such as biofilm systems or membrane bioreactors. In these systems, complex approaches based on partial derivative differential equations are proposed to model typical phenomena of diffusion or attachment/detachment [Eberl et al., 2006]).

Additionally, the idea of integration stressed by the European Water Framework Directive in relation to the management of water resources has also encouraged further advances in the mathematical modelling of wastewater treatment plants. Nowadays, the criteria for design, operation and control of WWTPs are still unit-process oriented; however, it has been demonstrated that optimum solutions can only be achieved when the interactions between the water and waste lines are considered. In this context, the term "Plant-Wide Modelling" is adopted to refer to all that work that, in the last years, has dealt with the integration of the existing unit-process models [Grau et al., 2007a]. Obviously, the WWTP design, operation and control problems become much more difficult and more time-consuming when they must be solved on the basis of plant-wide model approaches. Moreover, computational loads increase drastically with the application of modern methodologies where uncertainty analyses are included and, therefore, Monte Carlo simulations required [Benedetti et al., 2008].

Probably, the transfer of model-based methodologies from the academic domain to the water industry starts with the development and commercialisation of WWTP-specific simulation software packages such as WEST, SIMBA, GPS-X or Biowin. Though simulation has been traditionally addressed at supporting the design of WWTPs, interesting applications for operation and control have been also reported. Thus, based on combining historic data with dynamic simulations, Ayesa et al. [2001] implement a specific simulator for the Badiolegi WWTP that proves its effectiveness to facilitate both the diagnose of the plant and the exploration of operational strategies. Another example is the IWA/COST simulation benchmark, a simulation protocol which has been widely used to assess and compare control strategies [Coop, 2002]. Even so, current challenges are still focused on the establishment of systematic and straightforward procedures that assist in the proper use of modelling especially among practitioners and consultants. Thus, the goal for the coming years is to spread the use of simulation techniques in multiple areas: from industry to educational sectors. In this respect, two important barriers will have to be overcome: (1) the high investment built-in costs of simulation; and (2) model-based problem-solving is not a trivial issue, especially when optimum solutions are pursued.

Fortunately, the rapid consolidation of the World Wide Web as a common framework for applications has recently led to new web-based business models for accessing simulation services (web-based simulation). The distributed and client-server nature of the WWW enables: (1) the sharing of software resources between different customers so as to significantly reduce simulation costs; (2) hardware resources to be dedicated to specific simulation sub-tasks like processing, visualisation, storage, etc. Page and Opper [2000] classify web-based simulation practice into five primary areas: (1) simulation as hypermedia; (2) simulation research methodology; (3) web-based access to simulation programs; (4) Distributed modelling and simulation; and (5) Simulation of the WWW. Although several works dealing with each area have been reported in recent years, most of them cover area (3), i.e., web-based access to simulation programs. Wiedemann [2001] describes a web-based Application Service Provider for simulation of customised models and systems. By combining Java applet interfaces with distributed simulation, Yang and Alty [2002] demonstrate the potential of web-based online simulation for creating appropriate virtual experimental frameworks intended for distance learning. Cheng and Fen [2006] present a web-based distributed problem-solving platform for engineering applications. Additionally, the literature also reports some works on web-based simulation for wastewater treatment systems. For example, Samuelsson et al. [2001] employ Java applet technology to develop a Java-based dynamic simulator (JASS) for AS systems which can be accessed from any standard web browser.

There is a consensus around the necessity of model-based tools to cope with complex problems. However, these tools by themselves are not enough, being thus crucial to complement them with effective problem-solving methods that increase the confidence of end-users. Mathematical programming techniques represent valuable instruments in this concern, since their integration within model-based engineering problems allows optimum solutions to be found in an automatic way. These techniques have already been applied to specific AS configurations with satisfactory results [Rivas et al., 2008]. This success encourages their expansion to other wastewater treatments technologies and other unit-processes. By combining web-features and mathematical programming, this paper presents AqquaStudy, an Internet-based service that offers remote and free access to a library of software tools aimed at facilitating the optimum design and operation of WWTP unit-processes.

2. AQLIB: SOFTWARE LIBRARY OF MODEL-BASED OPTIMISATION TOOLS

So far, the utilisation of model-based software tools in the water industry has mainly concentrated on the dimensioning of conventional AS systems. Often, these tools are simply software implementations of systematic procedures such as the German ATV guidelines or similar [ATV, 2002]. Usually, model-based WWTP design combines steady-state and dynamic-state simulations: a preliminary steady-state study is carried out to estimate a first solution which, then, must be verified under non-steady conditions in order to refine the final solution. Within this two-step procedure, mathematical programming can help to automatically obtain optimum solutions for the steady-state problem. It is worth noting that the steady state of continuous flow systems corresponds to zero values for all time-derivatives; therefore, the steady-state condition becomes a non-linear algebraic equation system (instead of a differential one) that can be easily formulated and solved using mathematical optimisation tools. In contrast, concerning non-continuous technologies (e.g., SBR, Biodenitro, Biodenipho, intermittent systems …), their steady-state regime involves a periodic behaviour where time-derivatives get non-zero values. Consequently, a more different formulation is required for these technologies. Nevertheless, the application of optimisation techniques to these systems is beyond the scope of the present work.

AqLib, the software library of engineering tools described below, allows users to automatically solve studies under steady-state conditions. Rather than replacing current WWTP dynamic simulation software packages, the objective of AqLib is to complement them by providing initial estimations so as to facilitate subsequent studies under dynamic conditions. At present, only continuous flow technologies have been considered within AqLib, in particular: (1) seven AS configurations for nitrogen removal (DN, DN2, RDN, SDN, DRDN, RSDN and DRSDN); (2) five AS configurations for phosphorous removal (A^2O, Bardenpho, Johannesburg, UCT and MUCT); and (3) the anaerobic digestion process. Nevertheless, this library will be hopefully extended in the future to cover more configurations and more treatment technologies.

2. 1. Mathematical modelling and optimisation

Concerning the AS configurations, the standard ASM2d model was selected to describe the bio-chemical transformations in reactors. Moreover, a simple instantaneous settling model was set for secondary clarifiers: this model approach is good enough for steady-state studies focused on optimising the design/operation of biological tanks. In relation to the anaerobic digester software tool, it was based on the standard ADM1 model.

In general, the definition of an optimisation problem encompasses the three following items: (i) a cost function, whose value must approximate to a given objective; (ii) the independent variables that the mathematical programming algorithm can modify to reach the objective; and (iii) the constraints that the problem must satisfy. Thus, the mathematical algorithm searches the optimum values for the design/operation variables (volumes of anaerobic, anoxic, and aerated zones, internal recycling flow, waste flow, etc.) that comply with the problem constraints (maximum concentration of mixed liquor total suspended solids, minimum practical volumes, effluent quality, etc…). Values in Table 1 give, for the optimum design/operation problems of every configuration included in AqLib, an order of magnitude about their respective problem-solving complexity. The mathematical background around model-based optimisation algorithms for design and operation of WWTPs is detailed in Rivas et al. [2008]. Similarly, Irizar et al. [2005] and De Gracia et al. [2007] set out the equations involved in the development of a model-based optimisation software tool specific for the DN process and the anaerobic digester, respectively.

Table 1. Mathematical optimisation: built-in complexity of the optimum design/operation problems for different WW treatment technologies

	Nº of Independent Variables	Nº of Design/Operation Variables	Nº of Constraints
AS configurations for Nitrogen Removal			
DN	46	5	7
DN2	70	7	9
RDN	70	7	10
SDN	69	6	9
RSDN	92	8	10
DRDN	93	9	11
DRSDN	115	10	12
AS configurations for Phosphorous Removal			
A2O	69	6	9
Bardenpho	114	9	12
Johannesburg	92	8	10
UCT	70	7	9
MUCT	92	8	10
Sludge Treatment			
Anaerobic Digester	48	2	21

2. 2. Software implementation

Many mathematical problems can be easily formulated and solved through commercial spreadsheet packages. *Microsoft Excel* is probably the most widely-used spreadsheet by engineers. Although Excel is particularly appropriate when solving steady-state models, it also includes the VBA macro programming language so that dynamic models can also be solved. Moreover, *Solver* (by *Frontlyne Systems*, *Inc.*) is a commercial optimisation tool which is fully compatible with Excel in such a way that optimisation problems can be formulated within Excel worksheets before being solved through this tool. Therefore, since Excel meets the requirements for solving optimisation problems, AqLib has been implemented as a set of 13 Excel workbooks (one per treatment technology). All the workbooks have been designed in accordance to a unified pattern aimed at facilitating both their implementation and the development of additional model-based tools in the future. Thus, the 13 workbooks organise user information into four separated worksheets: (1) Influent characterisation; (2) Model coefficients; (3) Problem selection; and (4) Optimisation results. A screenshot of the "Influent Characterisation" worksheet for the DN tool is shown in Figure 1.

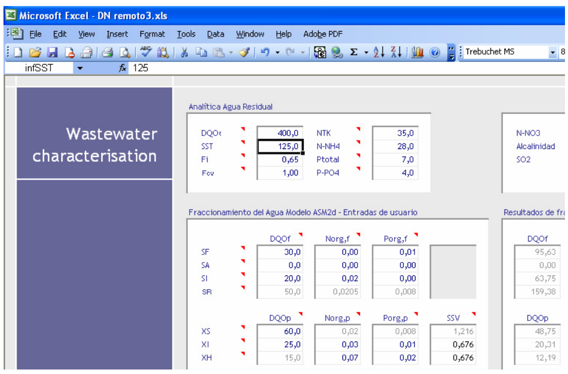

Figure 1. User input interface of the "Influent Characterisation" worksheet

In addition, every workbook includes a hidden worksheet where the design/operation problems are formulated in accordance to the specifications of the Solver optimisation tool. User-inputs in this worksheet are refreshed automatically every time a particular problem is launched to be solved. For that, within the workbook, specific VBA macros have been programmed that process user input information and send it to this worksheet before calling the Solver tool. Once the optimisation engine has solved the problem, these macros gather the solution and copy it to the "Optimisation Results" worksheet. In Figure 2, an overview of the software architecture of the implemented workbooks is illustrated.

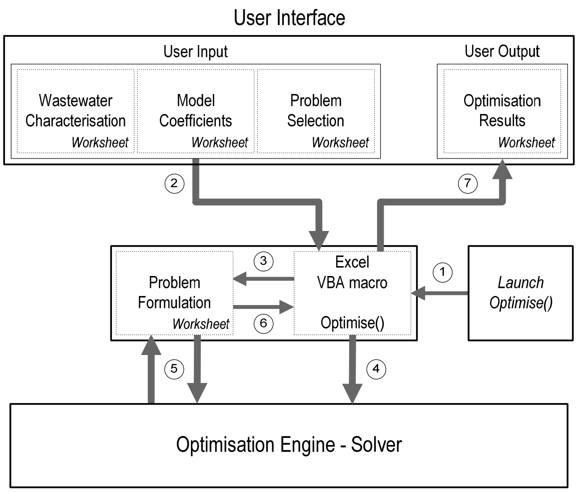

Figure 2. Software architecture of the Excel-based optimisation tools included in AqLib

3. AQQUASTUDY: INTERNET-BASED ACCESS TO THE SOFTWARE LIBRARY

Microsoft Excel integrates an OLE/COM interface that allows communication with external Windows-based applications supporting COM technology. This feature is especially attractive when the objective is to offer a remote service for accessing Excel-based engineering tools such as those contained in AqLib. The standard Web Services technology (http://www.w3.org/2002/ws/) has been used to implement a specific web service that provides client applications with a network interface for access to AqLib. The AqLib Web Service has been programmed within the Microsoft .NET environment because it supports COM technology. Through this web service, AqLib can be exploited by remote users from different client applications and hardware platforms. To achieve this, a XML schema has been defined so that clients and the web service can send each other I/O information bound to the problem-solving engineering tool. The web service architecture consists of three main layers: the interface layer; the logic layer; and the data access layer (Figure 3). Requests from clients are managed by the interface layer which dispatches them to the appropriate layer (either logic or data access). At the moment, four public functions form the interface layer:

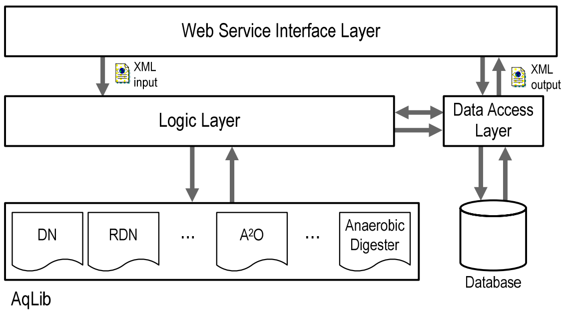

Figure 3. Architecture of the Web Service that enables remote access to AqLib

LaunchNewTask. Through this function clients invoke the web service in order for AqLib to solve a particular optimisation problem (task). *LaunchNewTask* requires two parameters from clients: (1) XML information defining the task (*XML task definition*); and (2) a *task Password* to protect access to task information. When this function is called, the interface layer sends both parameters to the logic layer and returns a *task Identifier* to the client.

IsTaskFinished. Clients make use of this function to know the current status (finished or in queue) of tasks launched previously. The function call has to include values for two parameters: *task Identifier* and *task Password*. An error code is returned if either parameter does not match correctly.

RemoveTask. Clients are able to remove tasks in the queue at any time by calling this function with the proper values for *task Identifier* and *task Password* arguments. Then, the interface layer sends this request to the data access layer for the removal of the task from the queue.

GetTaskSolution. Every time a task is solved by AqLib, the logic layer processes optimisation results (task results) and brings them in XML format to the data access layer. Finally, the data access layer stores the XML task results in the database. *GetTaskSolution* provides clients with a mechanism to gather XML task results. An e-mail address has been considered in the XML definition task structure so that the web service can alert users about the completion of their respective launched tasks.

3. 1. Web-based Client: AqquaStudy

As mentioned above, multiple client applications might be implemented in different hardware platforms for providing users with remote access to AqLib. Nevertheless, a default Web-based client application has been deployed that enables the AqLib tool to be used from any local computer connected to the Internet (Figure 4). This Web-based service has been named AqquaStudy (AqST) and, at present, it can be freely accessed from the web site http://www.aqquas.com (under construction). AqST represents a low-cost solution for small and medium water companies to incorporate modern WWTP design procedures. AqST enables new business models to be agreed such as pay per use instead of acquiring the software. Likewise, this service is aligned with current needs from workers who, because of a growing mobility, increasingly are demanding an access to software services from anywhere.

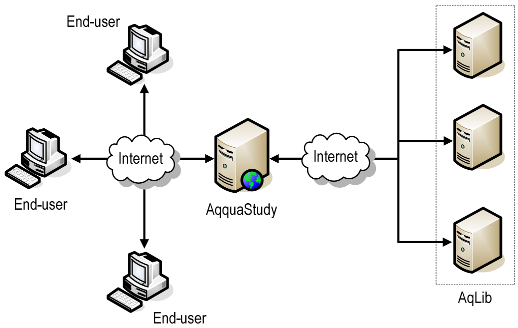

Figure 4. Hardware architecture of AqquaStudy

For now, AqST enables users to carry out model-based optimum design studies for three AS configurations: DN, DN2 and RDN. Figure 5 shows a screenshot of the user-input interface for the DN process. Initially, it has been designed a basic input interface where only the most relevant input information required to define an optimisation problem has been included. Thus, concerning the wastewater characteristics, only laboratory measurements have been considered (Total COD, Filtered COD, TSS, VSS, TKN and NH_4-N). On the other hand, default ratios have been used to obtain the different influent COD fractions, although this could be also optional for users depending on their knowledge. In addition, the following information is requested to define the optimisation problem: (1) temperature; (2) Mixed Liquor Suspended Solids in biological tanks; and (3) effluent Nitrogen requirements.

Figure 5. Screenshot of the Web-based user input interface for AqquaStudy: DN configuration

Similarly, a basic Web user output interface has been designed to give users the most significant optimisation results: (1) HRT and SRT; (2) Total Volume; (3) Anoxic and aerobic Volume fractions; (4) Internal recycling flow-rate; (5) Wasted sludge flow-rate; (6) Sludge production; (7) Oxygen requirements; and (8) Dissolved oxygen transfer coefficient in aerated tanks.

3. 2. System performance

An optimum design problem has been defined for the DN process in order to evaluate the performance of AqST (Table 2). This problem has been solved using two different tools: (1) AqST (AS); and (2) a commercial WWTP dynamic simulation software package (DS).

Table 2. Input data for the optimum design of the DN process

Wastewater Characteristics		
TCOD	mg O_2/L	350
FCOD	mg O_2/L	150
TSS	mg/L	125
VSS	mg/L	100
TKN	mg N/L	35
NH4-N	mg N/L	28
Design requirements		
Temperature	° C	15
MLSS	mg /L	3000
NH4-N	mg N/L	1
NO3-N	mg N/L	10

Table 3. Optimisation Results$^{(*)}$

		AqS	**DS**
HRT	h	13.9	13.8
SRT	d	14.2	14.1
Aerobic fraction	%	82	82
Internal Recycle	%Qinf	122	114
Waste Sludge	%Qinf	3.6	3.6
Effluent NH4-N	mg N/L	1	1
Effluent NO3-N	mg N/L	10	10
Solving Time	min	0.5	15-30

$^{(*)}$ Further details on the optimisation problem and the algorithm used can be found in Irizar et al. [2005]

Table 3 shows the results obtained with each tool. It can be seen that, in both cases, the optimum design was very similar. However, major differences appear when comparing the time consumed for reaching these results. While AqST took less than 1 minute to solve the problem, with the dynamic simulation tool, this value increased up to more than 15 minutes. In fact, these differences would have been more significant if the comparison, instead of using the DN process, had been done with a more complex configuration.

3. 3. Further extensions in AqquaStudy

The AqLib library should be extended in the next years with more engineering tools. Thus, further research must be addressed at incorporating additional problem-solving tools. Some examples are: (1) the design and operation of sequencing systems such as SBR, ATAD, etc.; (2) tools for wastewater characterisation [Grau et al., 2007b]; (3) the design of settling tanks; (4) the design of aeration systems, etc.

The hardware architecture of AqST can be easily expandable in the future depending on the end-user requirements. AqST supports the deployment of computational grids in the back-end (dedicated machines where the software applications of AqLib are installed) so as to increase both computational power and storage capacity and, as a consequence, to minimise the time for solving user-defined problems. At the moment, the XML task definition schema allows a single problem, only, to be specified. However, a new design for the XML task definition schema (and probably for the XML task results too) will have to be analysed for dealing with studies that demand batch simulations.

4. CONCLUSIONS

A software library has been designed for solving complex model-based engineering problems related to optimum design and operation of WWTP unit-processes. In addition, a Web-based approach (AqquaStudy) has been deployed to provide users with remote access to the software library. The implemented web service offers full utilisation of this tool from many different software clients as well as hardware platforms. AqquaStudy represents a valuable service to complement existing WWTP-specific dynamic simulation packages by providing them with the optimum values for the design/operation variables. Consequently, interfaces that automatically export the results from AqquaStudy to these commercial tools should be developed in order to facilitate users their utilisation.

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